

TOUGHREACT User's Guide: A Simulation Program for Non-isothermal Multiphase Reactive Geochemical Transport in Variably Saturated Geologic Media

Tianfu Xu, Eric Sonnenthal, Nicolas Spycher and Karsten Pruess

Earth Sciences Division, Lawrence Berkeley National Laboratory
University of California, Berkeley, CA 94720.

September 2004

This work was supported by the Laboratory Directed Research and Development Program of the Ernest Orlando Lawrence Berkeley National Laboratory; by the Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Geothermal Technologies; and by the Director, Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098.

TABLE OF CONTENTS

1. INTRODUCTION	1
2. REQUIREMENTS	3
2.1 Computer requirements and code installation	3
2.2 Memory requirements	3
2.3 User knowledge requirements	4
3. MODEL DESCRIPTION	5
3.1 Main scope of the model	5
3.2 Major processes	5
3.3 Governing equations	6
3.4 Simplifying approximations	7
4. SOLUTION METHOD	9
5. GENERAL DESCRIPTION OF INPUT AND OUTPUT FILES	13
5.1 Input Files	13
5.2 Output Files	14
5.2.1 Fixed-name output files	14
5.2.2 User-specified output files	15
6. INPUT FILE FORMATS AND CONTENTS	16
6.1 Flow input	16
6.2 Transport input	18
6.3 Geochemical input	24
6.4 Thermodynamic data	40

7. ANTICIPATED ERROR MESSAGES	45
8. SAMPLE PROBLEMS	48
8.1 Aqueous transport with adsorption (Linear Kd) and decay (EOS9)	48
8.2 Water quality in the Aquia aquifer, Maryland (EOS9)	54
8.3 Infiltration and calcite deposition at Yucca Mountain, Nevada (EOS3).....	61
8.4 Heater test problem (EOS4 or EOS3)	73
8.5 CO ₂ disposal in deep saline aquifers (ECO2)	88
8.6 Supergene copper enrichment (EOS9)	100
8.7 Caprock alteration (EOS2)	111
8.8 Injection well scaling and acidizing at Tiwi field, Philippines (EOS1)	119
9. CONCLUDING REMARKS	132
ACKNOWLEDGEMENTS	133
REFERENCES	133
APPENDIX A. Mathematical equations for flow and transport	146
APPENDIX B. Mathematical formulation of chemical reactions	148
APPENDIX C. Solution method for solute transport equations.....	158
C.1 Transport in the liquid phase	158
C.2 Transport in the gas phase	162
APPENDIX D. Solution method for mixed equilibrium-kinetics chemical system.....	164
APPENDIX E. Evaluation of the Jacobian matrix for chemical equations	168
APPENDIX F. Effects of mineral precipitation/dissolution on hydrologic properties ...	170
F.1 Porosity change	170
F.2 Fracture permeability change	170
F.3 Matrix permeability change	172
F.4 Effects of permeability and porosity changes on capillary pressures	173

APPENDIX G. Mineral reactive surface areas	174
APPENDIX H: Calculation of activity coefficients of aqueous species	177
APPENDIX I: Treatment for mineral solid solutions	185
APPENDIX J: Utility programs for chemical database	188
J.1. Converting EQ3/6 to TOUGHREACT database	188
J.2. Switching basis (primary) species	190
J.3. Regressing log(K) data	191
J.4. Checking mass and charge balances	192
Subject index	I